

2-METHYLHEXANEDIOIC ACID
33659-32-4 | DTXSID20334839

Model Performance

Model

Data

Weighted KNN model

| 5-fold CV (75%) | | Training (75%) | | Test (25%) | |
|-----------------|------|----------------|------|------------|------|
| Q2 | RMSE | R2 | RMSE | R2 | RMSE |
| 0.89 | 0.25 | 0.88 | 0.26 | 0.75 | 0.38 |

Model Results

Predicted value: 3.55 days

Global applicability domain: Outside

Local applicability domain index: 3.10e-01

Confidence level: 9.36e-01

Nearest Neighbors from the Training Set

| | | |
|---|---|---|
| <div>Image not found</div> <div>1-Methyl-2-propylbenzene</div> <div>Measured: 12.5</div> <div>Predicted: 3.17</div> | <div>Image not found</div> <div>Propylbenzene</div> <div>Measured: 24.3</div> <div>Predicted: 4.02</div> | <div>Image not found</div> <div>3-Ethyltoluene</div> <div>Measured: 12.5</div> <div>Predicted: 3.26</div> |
| <div>Image not found</div> <div>1-Ethyl-2-methylbenzene</div> <div>Measured: 24.3</div> <div>Predicted: 3.88</div> | <div>Image not found</div> <div>4-Ethyltoluene</div> <div>Measured: 24.3</div> <div>Predicted: 3.95</div> | |